Full wwPDB X-ray Structure Validation Report (i)

Sep 17, 2023 – 11:06 PM EDT

PDB ID	:	4Z90
Title	:	ELIC bound with the anesthetic isoflurane in the resting state
Authors	:	Chen, Q.; Kinde, M.; Arjunan, P.; Cohen, A.; Xu, Y.; Tang, P.
Deposited on	:	2015-04-09
Resolution	:	3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

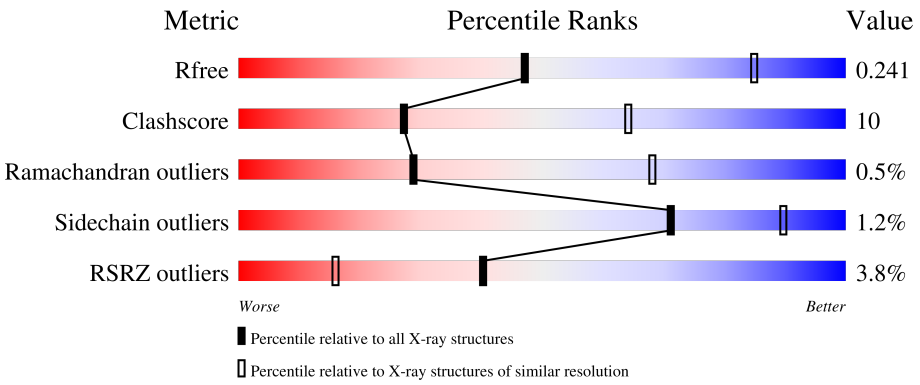
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	322	3% 77% 18% • •
1	B	322	3% 73% 22% • •
1	C	322	2% 74% 21% • •
1	D	322	4% 75% 19% • •
1	E	322	4% 75% 20% • •

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Mol	Chain	Length	Quality of chain
1	F	322	4% 73% 23%
1	G	322	2% 77% 18%
1	H	322	5% 69% 25%
1	I	322	4% 74% 22%
1	J	322	5% 69% 26%

2 Entry composition (i)

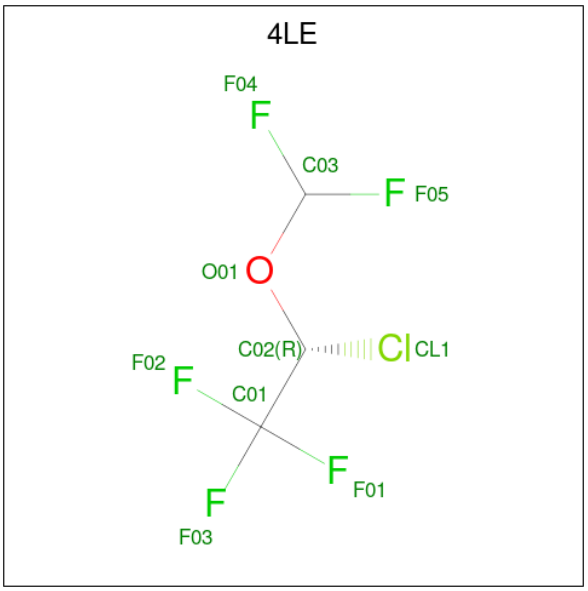
There are 4 unique types of molecules in this entry. The entry contains 25850 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Gamma-aminobutyric-acid receptor subunit beta-1.

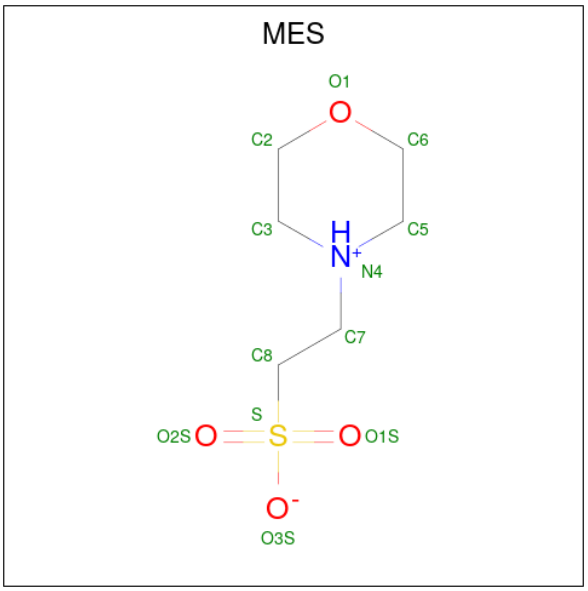
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	309	2527	1645	424	452	6	0	0	0
1	B	309	2527	1645	424	452	6	0	0	0
1	C	309	2527	1645	424	452	6	0	0	0
1	D	309	2527	1645	424	452	6	0	0	0
1	E	309	2527	1645	424	452	6	0	0	0
1	F	309	2527	1645	424	452	6	0	0	0
1	G	309	2527	1645	424	452	6	0	0	0
1	H	309	2527	1645	424	452	6	0	0	0
1	I	309	2527	1645	424	452	6	0	0	0
1	J	309	2527	1645	424	452	6	0	0	0

- Molecule 2 is (2R)-2-chloro-2-(difluoromethoxy)-1,1,1-trifluoroethane (three-letter code: 4LE) (formula: $C_3H_2ClF_5O$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Cl	F	O		
2	A	1	10	3	1	5	1	0	0
			Total	C	Cl	F	O		
2	E	1	10	3	1	5	1	0	0
			Total	C	Cl	F	O		
2	F	1	10	3	1	5	1	0	0
			Total	C	Cl	F	O		
2	F	1	10	3	1	5	1	0	0

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
3	A	1	12	6	1	4	1	0	0
			Total	C	N	O	S		
3	A	1	12	6	1	4	1	0	0
			Total	C	N	O	S		
3	B	1	12	6	1	4	1	0	0
			Total	C	N	O	S		
3	C	1	12	6	1	4	1	0	0
			Total	C	N	O	S		
3	D	1	12	6	1	4	1	0	0
			Total	C	N	O	S		
3	F	1	12	6	1	4	1	0	0
			Total	C	N	O	S		
3	G	1	12	6	1	4	1	0	0
			Total	C	N	O	S		
3	H	1	12	6	1	4	1	0	0
			Total	C	N	O	S		
3	I	1	12	6	1	4	1	0	0
			Total	C	N	O	S		
3	J	1	12	6	1	4	1	0	0

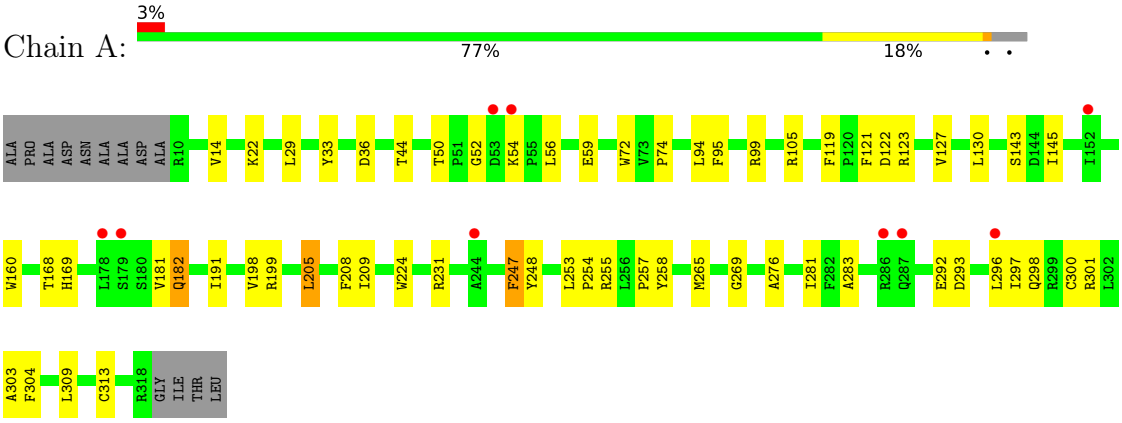
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	33	33	33	0	0
			Total	O		
4	B	45	45	45	0	0
			Total	O		
4	C	58	58	58	0	0
			Total	O		
4	D	30	30	30	0	0
			Total	O		
4	E	48	48	48	0	0
			Total	O		
4	F	33	33	33	0	0
			Total	O		
4	G	55	55	55	0	0
			Total	O		
4	H	42	42	42	0	0
			Total	O		
4	I	43	43	43	0	0
			Total	O		
4	J	33	33	33	0	0

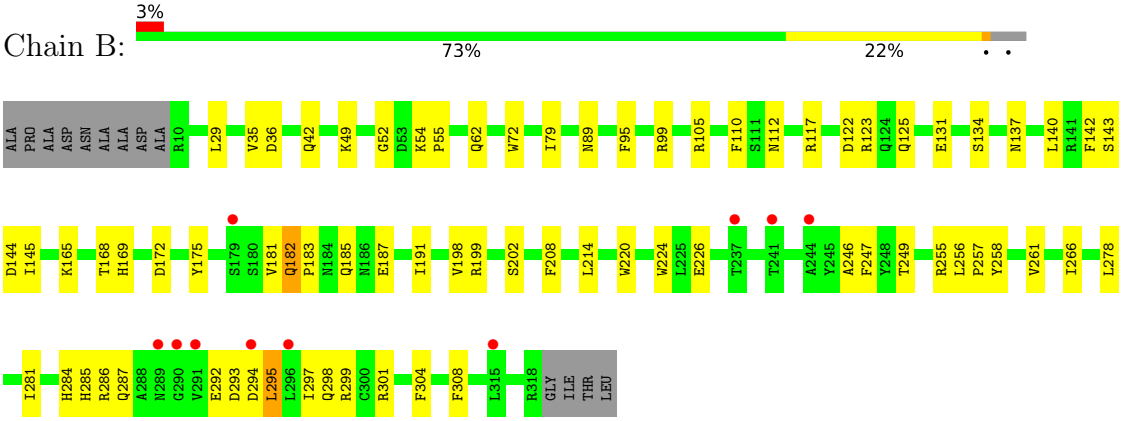
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

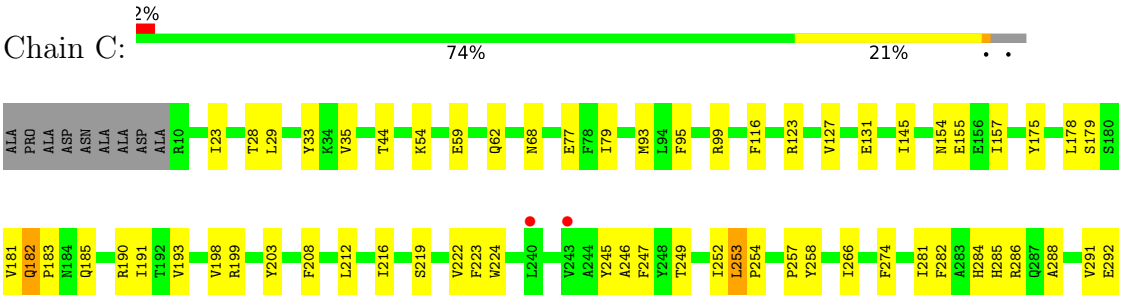
• Molecule 1: Gamma-aminobutyric-acid receptor subunit beta-1

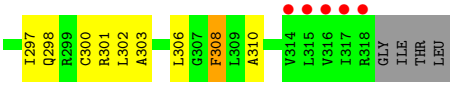


• Molecule 1: Gamma-aminobutyric-acid receptor subunit beta-1



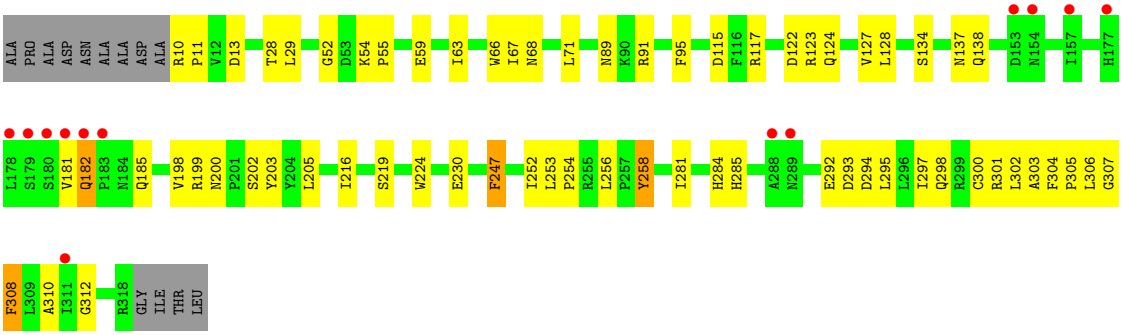
• Molecule 1: Gamma-aminobutyric-acid receptor subunit beta-1





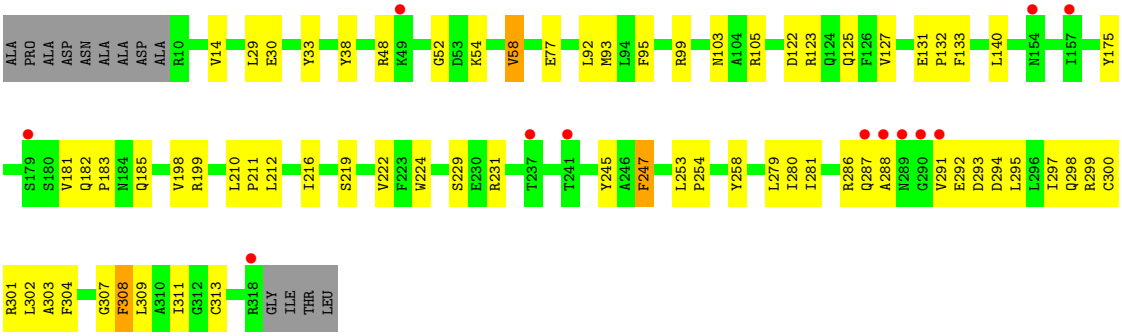
• Molecule 1: Gamma-aminobutyric-acid receptor subunit beta-1

Chain D:



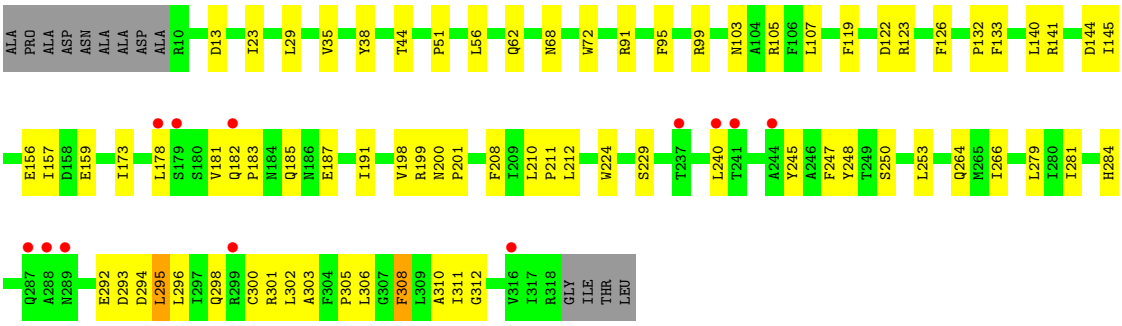
• Molecule 1: Gamma-aminobutyric-acid receptor subunit beta-1

Chain E:



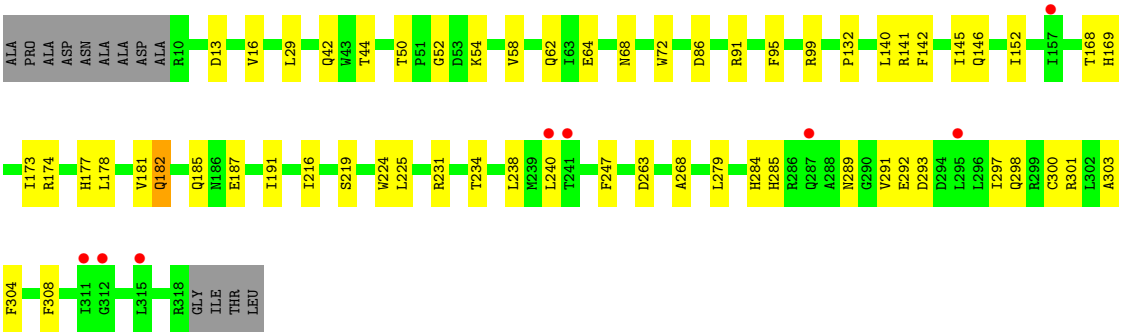
• Molecule 1: Gamma-aminobutyric-acid receptor subunit beta-1

Chain F:



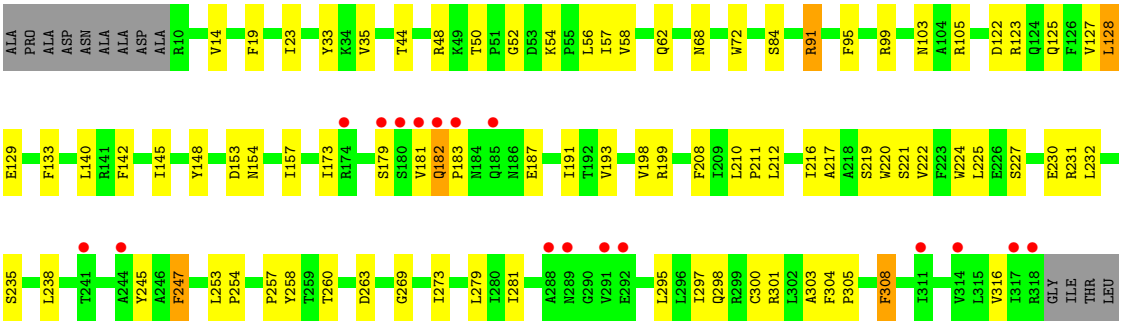
• Molecule 1: Gamma-aminobutyric-acid receptor subunit beta-1

Chain G:



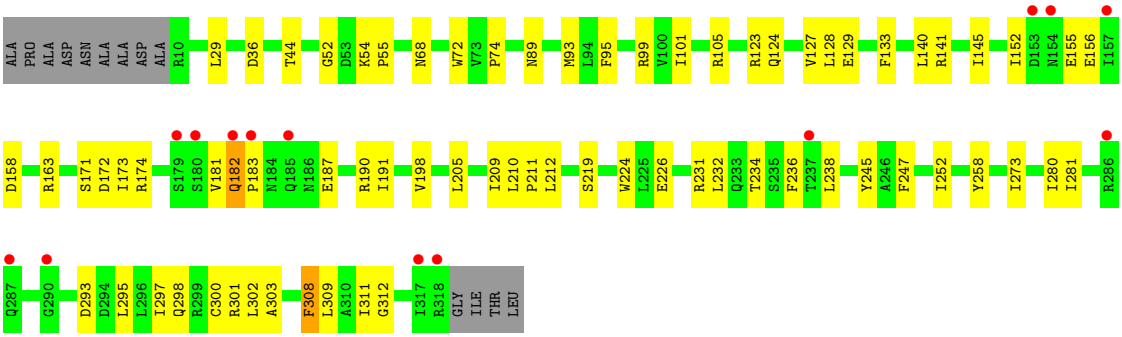
• Molecule 1: Gamma-aminobutyric-acid receptor subunit beta-1

Chain H:



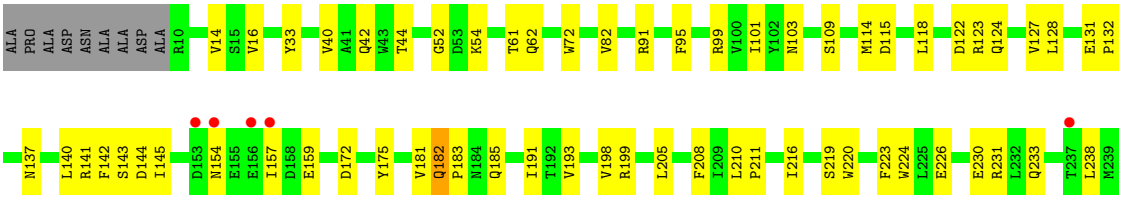
• Molecule 1: Gamma-aminobutyric-acid receptor subunit beta-1

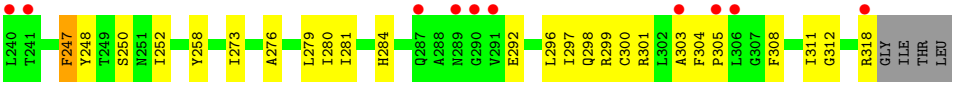
Chain I:



• Molecule 1: Gamma-aminobutyric-acid receptor subunit beta-1

Chain J:




L240
T241
F247
Y248
T249
S250
N251
I252
Y258
I273
A276
L279
I280
I281
H284
Q287
A288
N289
G290
V291
E292
L296
I297
Q298
R299
C300
R301
L302
A303
F304
P305
L306
G307
F308
I311
G312
R318
GLY
ILE
THR
LEU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	105.85Å 267.08Å 111.13Å 90.00° 106.94° 90.00°	Depositor
Resolution (Å)	36.97 – 3.00 39.63 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (36.97-3.00) 99.8 (39.63-3.00)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.75 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.209 , 0.243 0.210 , 0.241	Depositor DCC
R_{free} test set	5886 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	92.7	Xtriage
Anisotropy	0.343	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 61.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.024 for l,-k,h	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	25850	wwPDB-VP
Average B, all atoms (Å^2)	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.10% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MES, 4LE

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	A	0.61	0/2595	0.60	0/3536
1	B	0.73	0/2595	0.68	0/3536
1	C	0.71	0/2595	0.65	0/3536
1	D	0.81	0/2595	0.68	0/3536
1	E	0.66	0/2595	0.62	0/3536
1	F	0.59	0/2595	0.61	0/3536
1	G	0.74	0/2595	0.66	1/3536 (0.0%)
1	H	0.64	0/2595	0.65	1/3536 (0.0%)
1	I	0.68	0/2595	0.63	0/3536
1	J	0.55	0/2595	0.58	0/3536
All	All	0.68	0/25950	0.64	2/35360 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	128	LEU	CA-CB-CG	6.07	129.27	115.30
1	G	240	LEU	CA-CB-CG	5.30	127.50	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2527	0	2503	43	0
1	B	2527	0	2503	60	0
1	C	2527	0	2503	58	0
1	D	2527	0	2503	56	1
1	E	2527	0	2503	45	0
1	F	2527	0	2503	53	0
1	G	2527	0	2503	49	1
1	H	2527	0	2503	68	0
1	I	2527	0	2503	59	0
1	J	2527	0	2503	68	0
2	A	10	0	1	0	0
2	E	10	0	1	0	0
2	F	20	0	2	2	0
3	A	24	0	24	0	0
3	B	12	0	12	0	0
3	C	12	0	12	1	0
3	D	12	0	12	0	0
3	F	12	0	12	0	0
3	G	12	0	12	1	0
3	H	12	0	12	1	0
3	I	12	0	12	0	0
3	J	12	0	12	1	0
4	A	33	0	0	8	0
4	B	45	0	0	9	0
4	C	58	0	0	11	0
4	D	30	0	0	8	0
4	E	48	0	0	10	0
4	F	33	0	0	5	0
4	G	55	0	0	12	0
4	H	42	0	0	5	0
4	I	43	0	0	8	0
4	J	33	0	0	5	0
All	All	25850	0	25154	511	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (511) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:123:ARG:CG	1:D:198:VAL:HG12	1.79	1.11
1:B:79:ILE:HD11	1:B:131:GLU:HB3	1.24	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:123:ARG:HG2	1:D:198:VAL:CG1	1.82	1.07
1:I:123:ARG:CG	1:I:198:VAL:HG12	1.83	1.07
1:A:123:ARG:HG2	1:A:198:VAL:CG1	1.85	1.06
1:I:123:ARG:HG2	1:I:198:VAL:CG1	1.87	1.03
1:I:123:ARG:HG2	1:I:198:VAL:HG12	1.05	1.02
1:C:123:ARG:HG2	1:C:198:VAL:HG22	1.44	0.99
1:A:123:ARG:CG	1:A:198:VAL:HG12	1.93	0.98
1:H:123:ARG:HG2	1:H:198:VAL:HG22	1.46	0.97
1:D:123:ARG:HG2	1:D:198:VAL:HG12	0.98	0.95
1:B:79:ILE:HD11	1:B:131:GLU:CB	1.98	0.93
1:A:123:ARG:HG2	1:A:198:VAL:HG12	0.97	0.90
2:F:401:4LE:F05	2:F:401:4LE:CL1	2.17	0.87
1:H:257:PRO:O	4:H:501:HOH:O	1.92	0.87
1:E:30:GLU:OE1	4:E:501:HOH:O	1.95	0.85
1:B:79:ILE:CD1	1:B:131:GLU:HB3	2.06	0.84
1:C:62:GLN:NE2	1:D:68:ASN:OD1	2.12	0.83
1:G:91:ARG:NH1	4:G:503:HOH:O	2.12	0.82
1:E:123:ARG:HG2	1:E:198:VAL:HG12	1.60	0.82
1:J:16:VAL:HG11	1:J:191:ILE:CD1	2.10	0.81
1:B:187:GLU:OE2	1:I:141:ARG:NH1	2.13	0.79
1:C:190:ARG:NH2	4:C:501:HOH:O	2.14	0.79
1:H:316:VAL:HG12	1:H:316:VAL:O	1.83	0.79
1:E:293:ASP:O	4:E:502:HOH:O	2.00	0.79
1:I:232:LEU:HD22	1:I:281:ILE:HD11	1.64	0.79
1:J:118:LEU:HD21	1:J:318:ARG:HA	1.66	0.77
4:B:503:HOH:O	1:C:285:HIS:NE2	2.18	0.76
1:I:158:ASP:O	4:I:501:HOH:O	2.04	0.76
1:J:220:TRP:HZ2	1:J:308:PHE:HD2	1.33	0.76
1:G:132:PRO:O	4:G:501:HOH:O	2.03	0.76
1:C:131:GLU:OE1	4:C:501:HOH:O	2.05	0.74
1:H:129:GLU:OE2	4:H:502:HOH:O	2.05	0.74
1:G:231:ARG:NH2	1:G:292:GLU:OE2	2.21	0.73
1:C:79:ILE:O	4:C:502:HOH:O	2.06	0.73
1:J:44:THR:HA	1:J:99:ARG:HA	1.70	0.73
1:B:117:ARG:O	4:B:501:HOH:O	2.08	0.72
1:B:79:ILE:CD1	1:B:131:GLU:CB	2.67	0.72
1:C:284:HIS:HD2	1:C:292:GLU:HG2	1.55	0.72
1:E:48:ARG:NH1	4:E:505:HOH:O	2.23	0.72
1:A:59:GLU:OE2	4:A:501:HOH:O	2.08	0.71
1:D:284:HIS:ND1	1:D:292:GLU:OE1	2.24	0.71
1:I:155:GLU:OE1	4:I:502:HOH:O	2.07	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:125:GLN:OE1	4:E:503:HOH:O	2.07	0.71
1:F:123:ARG:HG2	1:F:198:VAL:HG12	1.71	0.71
1:G:42:GLN:OE1	1:H:179:SER:OG	2.07	0.71
1:G:263:ASP:OD2	4:G:502:HOH:O	2.08	0.71
1:J:284:HIS:ND1	1:J:292:GLU:OE1	2.19	0.71
1:B:168:THR:O	1:B:169:HIS:ND1	2.25	0.70
1:F:132:PRO:O	4:F:501:HOH:O	2.09	0.70
1:A:143:SER:N	4:A:503:HOH:O	2.24	0.70
1:I:226:GLU:OE2	1:J:284:HIS:NE2	2.25	0.70
1:D:13:ASP:O	4:D:501:HOH:O	2.10	0.69
1:D:181:VAL:HG22	1:D:182:GLN:H	1.57	0.69
1:A:14:VAL:N	4:A:503:HOH:O	2.25	0.68
1:H:181:VAL:HG22	1:H:182:GLN:H	1.58	0.68
1:J:123:ARG:HG2	1:J:198:VAL:HG22	1.75	0.68
1:C:127:VAL:HG23	1:C:193:VAL:O	1.93	0.68
1:D:59:GLU:OE2	4:D:503:HOH:O	2.12	0.68
1:H:99:ARG:O	4:H:503:HOH:O	2.10	0.68
1:G:177:HIS:ND1	4:G:509:HOH:O	2.27	0.67
1:E:287:GLN:NE2	1:E:293:ASP:OD1	2.27	0.67
1:D:137:ASN:OD1	4:D:502:HOH:O	2.11	0.67
1:C:203:TYR:N	4:C:507:HOH:O	2.27	0.66
1:G:181:VAL:HG22	1:G:182:GLN:H	1.60	0.66
1:H:224:TRP:CD2	1:H:301:ARG:HD2	2.30	0.66
1:J:61:THR:OG1	4:J:501:HOH:O	2.12	0.66
1:G:152:ILE:O	4:G:505:HOH:O	2.14	0.66
1:C:93:MET:SD	4:C:535:HOH:O	2.53	0.66
1:A:231:ARG:NH2	1:A:292:GLU:OE2	2.26	0.66
1:D:185:GLN:N	4:D:505:HOH:O	2.28	0.66
1:C:54:LYS:O	4:C:504:HOH:O	2.15	0.66
1:J:181:VAL:HG22	1:J:182:GLN:H	1.61	0.65
1:G:64:GLU:OE1	4:G:504:HOH:O	2.13	0.65
1:J:216:ILE:O	1:J:219:SER:OG	2.11	0.65
1:A:205:LEU:HD12	1:A:209:ILE:HG13	1.78	0.65
1:C:155:GLU:OE1	4:C:503:HOH:O	2.14	0.65
1:I:252:ILE:HD11	1:J:250:SER:HB2	1.79	0.65
1:F:145:ILE:HD13	1:F:191:ILE:HD13	1.78	0.65
1:I:224:TRP:CE2	1:I:301:ARG:HD3	2.32	0.65
1:B:226:GLU:OE2	4:B:503:HOH:O	2.14	0.64
1:G:289:ASN:HB2	1:G:291:VAL:HG12	1.79	0.64
1:C:224:TRP:CD2	1:C:301:ARG:HD2	2.33	0.64
1:E:132:PRO:HG3	1:E:140:LEU:HD22	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:16:VAL:CG1	1:J:191:ILE:CD1	2.75	0.64
1:A:122:ASP:OD1	1:A:199:ARG:NH1	2.31	0.64
1:H:62:GLN:NE2	1:I:68:ASN:OD1	2.29	0.64
1:J:141:ARG:NH2	4:J:506:HOH:O	2.31	0.64
1:F:44:THR:HA	1:F:99:ARG:HA	1.81	0.63
1:D:115:ASP:O	1:D:124:GLN:NE2	2.32	0.62
1:B:29:LEU:HD13	4:B:523:HOH:O	1.98	0.62
1:E:286:ARG:NH1	4:E:506:HOH:O	2.23	0.62
1:I:309:LEU:N	4:I:507:HOH:O	2.33	0.62
1:D:115:ASP:OD2	1:D:117:ARG:NH2	2.28	0.62
1:A:297:ILE:O	1:A:298:GLN:HB3	1.99	0.62
1:D:10:ARG:NH1	4:D:507:HOH:O	2.33	0.62
1:B:122:ASP:OD1	1:B:199:ARG:NH1	2.33	0.61
1:D:216:ILE:O	1:D:219:SER:HB3	2.00	0.61
1:I:308:PHE:HA	1:I:311:ILE:HG12	1.82	0.61
1:A:33:TYR:OH	1:A:127:VAL:N	2.29	0.61
1:C:59:GLU:OE2	1:D:134:SER:OG	2.13	0.61
1:C:145:ILE:HD13	1:C:191:ILE:HD13	1.81	0.61
1:G:62:GLN:NE2	1:H:68:ASN:OD1	2.29	0.61
1:H:182:GLN:HB2	1:H:183:PRO:HD3	1.82	0.60
1:F:298:GLN:HA	1:F:301:ARG:HG3	1.81	0.60
1:F:122:ASP:OD1	1:F:199:ARG:NH1	2.34	0.60
1:F:247:PHE:CD2	1:G:247:PHE:HE2	2.20	0.60
1:C:44:THR:HA	1:C:99:ARG:HA	1.83	0.59
1:J:131:GLU:OE2	1:J:175:TYR:OH	2.14	0.59
1:H:216:ILE:O	1:H:219:SER:OG	2.10	0.59
1:I:247:PHE:CD2	1:J:247:PHE:HE2	2.21	0.59
1:B:285:HIS:NE2	4:B:502:HOH:O	2.10	0.59
1:C:33:TYR:OH	1:C:127:VAL:O	2.20	0.59
1:A:44:THR:HA	1:A:99:ARG:HA	1.85	0.58
1:J:16:VAL:CG1	1:J:191:ILE:HD11	2.33	0.58
1:C:181:VAL:HG12	1:C:182:GLN:H	1.67	0.58
1:C:284:HIS:CD2	1:C:292:GLU:HG2	2.38	0.58
1:A:160:TRP:O	4:A:502:HOH:O	2.17	0.58
1:I:174:ARG:NH1	4:I:509:HOH:O	2.35	0.58
1:H:142:PHE:CD2	1:H:191:ILE:HG13	2.39	0.58
1:A:283:ALA:HB2	1:A:296:LEU:HD23	1.85	0.58
1:A:224:TRP:CE2	1:A:301:ARG:HD3	2.39	0.57
1:D:306:LEU:O	1:D:310:ALA:N	2.37	0.57
1:D:247:PHE:CD2	1:E:247:PHE:HE2	2.21	0.57
1:I:231:ARG:HB3	1:I:280:ILE:HD13	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:300:CYS:HA	1:J:303:ALA:HB3	1.85	0.57
1:C:99:ARG:O	4:C:505:HOH:O	2.16	0.57
1:F:306:LEU:O	1:F:310:ALA:N	2.37	0.57
1:H:19:PHE:CE2	1:H:148:TYR:HD2	2.22	0.57
1:C:33:TYR:OH	1:C:127:VAL:N	2.37	0.57
1:J:137:ASN:ND2	1:J:172:ASP:OD2	2.36	0.57
4:G:503:HOH:O	1:H:133:PHE:O	2.18	0.57
1:B:131:GLU:OE2	1:B:175:TYR:OH	2.14	0.57
1:I:124:GLN:OE1	4:I:504:HOH:O	2.17	0.57
1:J:16:VAL:HG11	1:J:191:ILE:HD11	1.87	0.57
1:J:279:LEU:HD23	1:J:300:CYS:SG	2.44	0.57
1:B:42:GLN:OE1	1:C:179:SER:OG	2.14	0.57
1:B:208:PHE:HE1	1:B:249:THR:HA	1.69	0.56
1:B:62:GLN:NE2	1:C:68:ASN:OD1	2.31	0.56
1:B:168:THR:C	1:B:169:HIS:ND1	2.59	0.56
1:H:316:VAL:O	1:H:316:VAL:CG1	2.53	0.56
1:I:182:GLN:HB2	1:I:183:PRO:HD3	1.87	0.56
1:G:225:LEU:HB2	1:G:231:ARG:HG2	1.87	0.56
1:H:44:THR:HA	1:H:99:ARG:HA	1.87	0.56
1:I:89:ASN:ND2	4:I:503:HOH:O	2.09	0.56
1:J:16:VAL:HG23	1:J:40:VAL:O	2.06	0.56
1:B:137:ASN:ND2	1:B:172:ASP:OD2	2.38	0.56
1:A:181:VAL:HG12	1:A:182:GLN:H	1.71	0.56
1:B:123:ARG:HG2	1:B:198:VAL:HG23	1.88	0.56
1:H:33:TYR:OH	1:H:127:VAL:N	2.36	0.56
1:E:77:GLU:OE2	4:E:504:HOH:O	2.18	0.56
1:H:154:ASN:O	1:H:157:ILE:HG12	2.07	0.55
1:G:13:ASP:OD1	1:G:141:ARG:NH1	2.40	0.55
1:B:143:SER:OG	1:B:144:ASP:OD2	2.24	0.55
1:C:252:ILE:HG12	4:C:534:HOH:O	2.07	0.55
1:F:212:LEU:HD12	1:F:245:TYR:CE2	2.41	0.55
1:G:72:TRP:HH2	1:G:140:LEU:HD12	1.70	0.55
1:B:208:PHE:CD1	1:B:249:THR:HG22	2.42	0.55
1:E:183:PRO:O	1:E:185:GLN:HG2	2.07	0.55
1:D:300:CYS:HA	1:D:303:ALA:HB3	1.89	0.55
1:B:224:TRP:CE2	1:B:301:ARG:HD3	2.42	0.54
1:B:247:PHE:CD1	1:C:247:PHE:HE2	2.25	0.54
1:E:122:ASP:OD2	1:E:199:ARG:NH1	2.40	0.54
1:J:238:LEU:HB3	1:J:273:ILE:HD12	1.90	0.54
1:F:293:ASP:OD1	1:F:296:LEU:N	2.36	0.54
1:B:284:HIS:ND1	1:B:292:GLU:HG2	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:72:TRP:CH2	1:B:140:LEU:HD12	2.42	0.54
1:A:121:PHE:HZ	1:A:205:LEU:HD11	1.72	0.54
1:I:55:PRO:HB3	1:I:95:PHE:CD2	2.43	0.54
1:B:181:VAL:HG12	1:B:182:GLN:H	1.72	0.54
1:D:122:ASP:OD1	1:D:199:ARG:NH1	2.40	0.54
1:I:300:CYS:HA	1:I:303:ALA:HB3	1.90	0.54
1:E:95:PHE:HB2	1:E:99:ARG:HG3	1.90	0.53
1:H:128:LEU:HB2	1:H:193:VAL:HG22	1.90	0.53
1:A:300:CYS:HA	1:A:303:ALA:HB3	1.91	0.53
1:I:219:SER:HA	1:I:238:LEU:HD13	1.90	0.53
1:J:95:PHE:HB2	1:J:99:ARG:HG3	1.90	0.53
1:B:95:PHE:HB2	1:B:99:ARG:HG3	1.89	0.53
1:D:202:SER:OG	1:D:203:TYR:N	2.41	0.53
1:E:309:LEU:O	1:E:313:CYS:HB2	2.09	0.53
1:I:210:LEU:HB3	1:I:211:PRO:HD3	1.90	0.53
1:J:297:ILE:O	1:J:298:GLN:HB3	2.09	0.53
1:A:247:PHE:HE2	1:E:247:PHE:CD2	2.26	0.53
1:F:95:PHE:HB2	1:F:99:ARG:HG3	1.90	0.53
1:G:44:THR:HA	1:G:99:ARG:HA	1.90	0.53
1:G:279:LEU:HD23	1:G:300:CYS:SG	2.48	0.53
1:I:205:LEU:HD23	1:I:209:ILE:HG13	1.89	0.53
1:G:297:ILE:O	1:G:298:GLN:HB3	2.09	0.52
1:C:253:LEU:HB3	1:C:254:PRO:HD2	1.90	0.52
1:E:131:GLU:OE2	1:E:175:TYR:OH	2.14	0.52
1:E:297:ILE:O	1:E:298:GLN:HB3	2.08	0.52
1:E:103:ASN:ND2	4:E:515:HOH:O	2.42	0.52
1:E:216:ILE:O	1:E:219:SER:HB3	2.09	0.52
1:D:224:TRP:CE2	1:D:301:ARG:HD3	2.44	0.52
1:B:298:GLN:HA	1:B:301:ARG:HG3	1.91	0.52
1:J:115:ASP:O	1:J:124:GLN:NE2	2.41	0.52
1:H:33:TYR:OH	1:H:127:VAL:O	2.25	0.52
1:H:95:PHE:HB2	1:H:99:ARG:HG3	1.91	0.52
1:F:133:PHE:HE2	1:J:91:ARG:HB2	1.74	0.52
1:E:224:TRP:CE2	1:E:301:ARG:HD3	2.45	0.51
1:E:299:ARG:NH1	4:E:506:HOH:O	2.42	0.51
1:E:231:ARG:HB3	1:E:280:ILE:HD13	1.93	0.51
3:G:401:MES:O2S	4:G:506:HOH:O	2.18	0.51
1:G:146:GLN:N	4:G:512:HOH:O	2.43	0.51
1:H:125:GLN:N	4:H:507:HOH:O	2.28	0.51
1:F:308:PHE:HA	1:F:311:ILE:HG13	1.91	0.51
1:H:238:LEU:HB3	1:H:273:ILE:HD12	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:288:ALA:O	1:E:291:VAL:HG12	2.10	0.51
1:J:154:ASN:O	1:J:157:ILE:HG12	2.11	0.51
1:E:33:TYR:OH	1:E:127:VAL:N	2.38	0.51
1:A:22:LYS:NZ	4:A:510:HOH:O	2.43	0.51
1:C:298:GLN:HG3	1:C:301:ARG:NH2	2.26	0.51
1:I:152:ILE:O	4:I:505:HOH:O	2.20	0.50
1:F:91:ARG:NH1	1:F:103:ASN:HD22	2.09	0.50
1:F:302:LEU:HA	1:F:305:PRO:HG2	1.93	0.50
1:D:55:PRO:HB3	1:D:95:PHE:CD2	2.47	0.50
1:J:276:ALA:HB2	1:J:304:PHE:HE2	1.76	0.50
1:E:58:VAL:HG13	1:E:92:LEU:HB2	1.93	0.50
1:G:72:TRP:CH2	1:G:140:LEU:HD12	2.46	0.50
1:J:72:TRP:HH2	1:J:140:LEU:HD12	1.77	0.50
4:A:501:HOH:O	1:B:134:SER:N	2.43	0.50
1:E:224:TRP:CD2	1:E:301:ARG:HD3	2.47	0.50
1:F:279:LEU:HD23	1:F:300:CYS:SG	2.52	0.50
1:I:298:GLN:HA	1:I:301:ARG:HG3	1.93	0.50
1:J:82:VAL:N	1:J:109:SER:O	2.38	0.50
1:A:145:ILE:HG23	1:A:168:THR:HG21	1.93	0.50
1:F:51:PRO:HD2	1:F:56:LEU:HD12	1.93	0.50
1:H:52:GLY:C	1:H:54:LYS:H	2.15	0.50
1:H:212:LEU:HD13	1:H:245:TYR:CD2	2.46	0.50
1:D:298:GLN:HA	1:D:301:ARG:HG3	1.94	0.50
1:I:247:PHE:CD2	1:J:247:PHE:CE2	2.99	0.50
1:H:173:ILE:O	1:H:187:GLU:HA	2.12	0.49
1:J:91:ARG:CZ	1:J:103:ASN:HD22	2.25	0.49
1:H:50:THR:OG1	1:H:52:GLY:O	2.30	0.49
1:A:50:THR:OG1	1:A:52:GLY:O	2.30	0.49
1:G:284:HIS:O	1:G:285:HIS:HD2	1.96	0.49
1:H:247:PHE:CD2	1:I:247:PHE:HE2	2.30	0.49
3:J:401:MES:O1S	4:J:502:HOH:O	2.19	0.49
1:A:95:PHE:HB2	1:A:99:ARG:HG3	1.95	0.49
1:A:255:ARG:NE	4:A:511:HOH:O	2.44	0.49
1:J:183:PRO:O	1:J:185:GLN:HG2	2.13	0.49
1:G:132:PRO:CG	1:G:140:LEU:HD22	2.43	0.49
1:I:308:PHE:O	1:I:312:GLY:N	2.46	0.49
1:A:247:PHE:CD2	1:B:247:PHE:HE1	2.31	0.49
1:C:216:ILE:O	1:C:219:SER:OG	2.29	0.49
1:C:219:SER:O	1:C:222:VAL:HG23	2.12	0.49
1:G:268:ALA:HB1	1:G:308:PHE:CE1	2.48	0.49
1:J:114:MET:O	4:J:503:HOH:O	2.19	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:36:ASP:OD2	1:B:105:ARG:NH2	2.36	0.49
1:B:105:ARG:NH1	4:C:502:HOH:O	2.46	0.49
1:B:220:TRP:HZ2	1:B:308:PHE:CD2	2.31	0.49
1:H:219:SER:O	1:H:222:VAL:HG23	2.12	0.49
1:F:308:PHE:O	1:F:312:GLY:N	2.45	0.48
1:I:93:MET:HE3	1:I:101:ILE:HD12	1.95	0.48
1:J:140:LEU:O	4:J:504:HOH:O	2.20	0.48
1:H:122:ASP:OD1	1:H:199:ARG:NH1	2.47	0.48
1:H:219:SER:HB2	1:H:238:LEU:HD23	1.95	0.48
1:B:292:GLU:O	1:B:294:ASP:N	2.47	0.48
1:D:230:GLU:OE2	1:E:229:SER:OG	2.20	0.48
1:A:257:PRO:HG2	1:A:258:TYR:CD2	2.49	0.48
1:A:309:LEU:O	1:A:313:CYS:HB2	2.14	0.48
1:C:247:PHE:CD2	1:D:247:PHE:HE2	2.32	0.48
4:F:503:HOH:O	1:J:99:ARG:NH1	2.47	0.48
1:H:145:ILE:HD13	1:H:191:ILE:HD13	1.96	0.48
1:I:36:ASP:OD1	1:I:105:ARG:NH2	2.46	0.48
1:G:99:ARG:O	4:G:507:HOH:O	2.20	0.48
1:C:29:LEU:HB2	4:C:528:HOH:O	2.13	0.47
1:G:247:PHE:CD2	1:H:247:PHE:HE2	2.31	0.47
1:B:72:TRP:HH2	1:B:140:LEU:HD12	1.79	0.47
1:B:165:LYS:HG3	1:I:163:ARG:HG2	1.95	0.47
1:D:224:TRP:CG	1:E:281:ILE:HD11	2.49	0.47
1:J:231:ARG:HB3	1:J:280:ILE:HD13	1.96	0.47
1:E:300:CYS:HA	1:E:303:ALA:HB3	1.96	0.47
1:F:68:ASN:OD1	1:J:62:GLN:NE2	2.32	0.47
1:F:119:PHE:CE1	1:F:253:LEU:HD22	2.49	0.47
1:A:208:PHE:CE1	1:A:248:TYR:CE2	3.02	0.47
1:D:200:ASN:O	4:D:504:HOH:O	2.20	0.47
1:H:198:VAL:HG12	1:H:199:ARG:N	2.30	0.47
1:D:138:GLN:HG3	1:D:185:GLN:NE2	2.30	0.47
1:D:202:SER:OG	4:D:504:HOH:O	2.21	0.47
1:J:132:PRO:HD3	1:J:142:PHE:CE2	2.49	0.47
1:B:224:TRP:CD2	1:B:301:ARG:HD3	2.50	0.47
1:H:298:GLN:HG3	1:H:301:ARG:NH2	2.30	0.47
1:J:72:TRP:CH2	1:J:140:LEU:HD12	2.50	0.47
1:B:55:PRO:HB3	1:B:95:PHE:CD2	2.50	0.47
1:D:10:ARG:HB3	1:D:11:PRO:HD3	1.97	0.47
1:F:62:GLN:NE2	1:G:68:ASN:OD1	2.44	0.47
1:A:224:TRP:CD2	1:A:301:ARG:HD3	2.51	0.46
1:B:112:ASN:ND2	1:B:125:GLN:O	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:145:ILE:HD13	1:I:191:ILE:HG21	1.97	0.46
1:A:281:ILE:HD11	1:E:224:TRP:HB2	1.97	0.46
1:F:208:PHE:HE1	1:F:248:TYR:CZ	2.33	0.46
1:H:308:PHE:C	1:H:308:PHE:CD2	2.88	0.46
1:I:133:PHE:N	4:I:510:HOH:O	2.48	0.46
1:I:173:ILE:O	1:I:187:GLU:HA	2.15	0.46
1:C:300:CYS:HA	1:C:303:ALA:HB3	1.98	0.46
1:E:93:MET:HB2	4:E:519:HOH:O	2.15	0.46
1:E:307:GLY:O	1:E:311:ILE:HG12	2.16	0.46
1:E:308:PHE:C	1:E:308:PHE:CD2	2.89	0.46
1:D:297:ILE:O	1:D:298:GLN:HB2	2.15	0.46
1:F:72:TRP:CH2	1:F:140:LEU:HD12	2.50	0.46
1:F:250:SER:HB2	1:J:252:ILE:HD11	1.98	0.46
1:F:264:GLN:NE2	4:F:506:HOH:O	2.49	0.46
1:I:44:THR:HA	1:I:99:ARG:HA	1.97	0.46
1:I:234:THR:HG1	1:J:233:GLN:HE21	1.57	0.46
1:D:303:ALA:O	1:D:307:GLY:N	2.36	0.46
1:C:23:ILE:HG12	1:C:35:VAL:HG22	1.98	0.46
1:F:23:ILE:HG21	1:F:126:PHE:CD2	2.51	0.46
1:B:142:PHE:CD2	1:B:191:ILE:HG13	2.50	0.46
1:E:210:LEU:HB3	1:E:211:PRO:HD3	1.97	0.46
1:F:133:PHE:CE2	1:J:91:ARG:HB2	2.50	0.46
1:B:89:ASN:ND2	4:B:505:HOH:O	2.20	0.46
1:A:253:LEU:HB3	1:A:254:PRO:HD2	1.98	0.45
1:E:52:GLY:C	1:E:54:LYS:H	2.18	0.45
1:F:240:LEU:HD11	2:F:402:4LE:F01	2.06	0.45
1:F:300:CYS:HA	1:F:303:ALA:HB3	1.98	0.45
1:F:308:PHE:CD2	1:F:308:PHE:C	2.89	0.45
1:I:171:SER:OG	1:I:172:ASP:N	2.48	0.45
1:H:14:VAL:HG13	1:H:142:PHE:HD1	1.82	0.45
1:F:173:ILE:O	1:F:187:GLU:HA	2.17	0.45
1:H:279:LEU:HD23	1:H:300:CYS:SG	2.56	0.45
1:I:234:THR:OG1	1:J:233:GLN:NE2	2.40	0.45
1:C:183:PRO:O	1:C:185:GLN:HG2	2.16	0.45
1:D:63:ILE:O	1:D:67:ILE:HG12	2.16	0.45
1:F:144:ASP:HB2	4:F:505:HOH:O	2.17	0.45
1:F:210:LEU:HB3	1:F:211:PRO:HD3	1.99	0.45
1:G:146:GLN:HG2	4:G:512:HOH:O	2.15	0.45
1:J:308:PHE:O	1:J:312:GLY:N	2.50	0.45
1:J:220:TRP:CZ3	1:J:305:PRO:HA	2.51	0.45
1:A:72:TRP:CH2	1:A:74:PRO:HG3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:282:PHE:CZ	1:C:286:ARG:HG3	2.52	0.45
1:D:253:LEU:HB3	1:D:254:PRO:HD2	1.98	0.45
1:A:119:PHE:CE1	1:A:253:LEU:HD22	2.52	0.45
1:G:234:THR:O	1:G:238:LEU:HD13	2.17	0.45
1:G:285:HIS:HA	4:G:530:HOH:O	2.16	0.45
1:H:91:ARG:NH1	1:H:103:ASN:HD22	2.15	0.45
1:B:246:ALA:HA	1:B:266:ILE:HD13	1.98	0.45
1:E:222:VAL:O	1:E:231:ARG:HG2	2.17	0.45
1:B:79:ILE:CD1	1:B:131:GLU:HB2	2.47	0.45
1:F:13:ASP:OD1	1:F:141:ARG:NH1	2.49	0.45
1:G:95:PHE:HB2	1:G:99:ARG:HG3	1.98	0.45
1:H:300:CYS:HA	1:H:303:ALA:HB3	1.99	0.45
1:J:308:PHE:HA	1:J:311:ILE:HG22	1.99	0.45
1:F:281:ILE:HD11	1:J:224:TRP:CG	2.52	0.45
1:H:227:SER:O	1:H:231:ARG:HG3	2.16	0.45
1:I:224:TRP:CG	1:J:281:ILE:HD11	2.52	0.45
1:C:224:TRP:CE2	1:C:301:ARG:HD2	2.52	0.44
1:C:224:TRP:CG	1:D:281:ILE:HD11	2.52	0.44
1:F:183:PRO:O	1:F:185:GLN:HG2	2.17	0.44
1:J:42:GLN:HG3	1:J:101:ILE:HG12	1.99	0.44
1:A:36:ASP:CG	1:A:105:ARG:HH21	2.20	0.44
1:A:224:TRP:CG	1:B:281:ILE:HD11	2.53	0.44
1:B:298:GLN:HG2	1:B:301:ARG:NH2	2.32	0.44
1:E:292:GLU:O	1:E:294:ASP:N	2.50	0.44
1:F:284:HIS:NE2	1:J:226:GLU:OE2	2.40	0.44
1:J:122:ASP:OD1	1:J:199:ARG:NH1	2.51	0.44
1:C:95:PHE:HB2	1:C:99:ARG:HG3	1.99	0.44
1:F:156:GLU:HG2	1:F:157:ILE:HG23	1.99	0.44
1:J:298:GLN:HA	1:J:301:ARG:HG3	1.98	0.44
1:B:278:LEU:O	1:B:281:ILE:HG22	2.17	0.44
1:F:29:LEU:HD21	1:J:159:GLU:OE2	2.17	0.44
1:F:35:VAL:O	1:F:107:LEU:HD12	2.18	0.44
1:G:279:LEU:HD22	1:G:304:PHE:CZ	2.53	0.44
1:I:29:LEU:HA	1:I:29:LEU:HD23	1.75	0.44
1:B:145:ILE:HD13	1:B:191:ILE:HD13	1.99	0.44
1:C:154:ASN:O	1:C:157:ILE:HG12	2.17	0.44
1:C:306:LEU:O	1:C:310:ALA:N	2.50	0.44
1:D:284:HIS:O	1:D:285:HIS:HD2	2.00	0.44
1:F:224:TRP:CE2	1:F:301:ARG:HD3	2.53	0.44
1:G:52:GLY:C	1:G:54:LYS:H	2.20	0.44
1:D:89:ASN:HB2	1:E:133:PHE:CE1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:212:LEU:HD23	1:E:245:TYR:CD2	2.52	0.43
1:J:52:GLY:C	1:J:54:LYS:H	2.20	0.43
1:A:265:MET:O	1:A:269:GLY:N	2.47	0.43
1:B:255:ARG:O	1:B:256:LEU:HD12	2.18	0.43
1:D:292:GLU:O	1:D:294:ASP:N	2.51	0.43
1:H:304:PHE:HB2	1:H:305:PRO:HD3	2.00	0.43
1:J:296:LEU:O	1:J:299:ARG:HB2	2.18	0.43
1:C:208:PHE:CD1	1:C:249:THR:HG22	2.52	0.43
1:H:298:GLN:HA	1:H:301:ARG:HG3	1.99	0.43
1:F:293:ASP:C	1:F:295:LEU:H	2.22	0.43
1:G:132:PRO:HG3	1:G:140:LEU:HD22	2.00	0.43
1:H:297:ILE:O	1:H:298:GLN:HB3	2.19	0.43
1:I:238:LEU:HB3	1:I:273:ILE:HD13	2.00	0.43
1:B:52:GLY:C	1:B:54:LYS:H	2.21	0.43
1:B:286:ARG:HD3	1:B:287:GLN:HG3	2.00	0.43
1:D:123:ARG:CD	1:D:198:VAL:HG12	2.46	0.43
1:H:48:ARG:NH1	4:H:503:HOH:O	2.51	0.43
1:J:14:VAL:HG11	1:J:140:LEU:HD21	2.00	0.43
1:D:293:ASP:OD1	1:D:295:LEU:HB3	2.19	0.43
1:B:49:LYS:HA	4:B:514:HOH:O	2.18	0.43
1:F:247:PHE:HE2	1:J:247:PHE:CD2	2.37	0.43
1:G:173:ILE:O	1:G:187:GLU:HA	2.19	0.43
1:I:36:ASP:CG	1:I:105:ARG:HH21	2.22	0.43
1:I:156:GLU:OE1	1:I:156:GLU:N	2.52	0.43
1:A:276:ALA:HB2	1:A:304:PHE:HE2	1.82	0.43
1:B:257:PRO:HG2	1:B:258:TYR:CD2	2.54	0.43
1:C:308:PHE:C	1:C:308:PHE:CD2	2.91	0.43
1:D:205:LEU:HD23	1:D:205:LEU:HA	1.65	0.43
1:H:23:ILE:HG12	1:H:35:VAL:HG22	2.01	0.43
1:J:210:LEU:HB3	1:J:211:PRO:HD3	1.99	0.43
1:B:214:LEU:HD23	1:B:214:LEU:HA	1.78	0.42
1:D:28:THR:HG21	1:D:254:PRO:HB2	2.01	0.42
1:D:252:ILE:HD13	4:D:509:HOH:O	2.18	0.42
1:D:302:LEU:HD23	1:D:302:LEU:HA	1.85	0.42
1:G:224:TRP:CE2	1:G:301:ARG:HD3	2.54	0.42
1:I:298:GLN:HG2	1:I:301:ARG:CZ	2.49	0.42
1:J:33:TYR:OH	1:J:127:VAL:N	2.41	0.42
1:C:297:ILE:O	1:C:298:GLN:HB3	2.19	0.42
1:G:300:CYS:HA	1:G:303:ALA:HB3	2.01	0.42
1:H:128:LEU:HB2	1:H:193:VAL:CG2	2.49	0.42
1:H:253:LEU:HB3	1:H:254:PRO:HD2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:261:VAL:HG23	4:B:501:HOH:O	2.19	0.42
1:D:304:PHE:HB2	1:D:305:PRO:HD3	2.01	0.42
1:H:153:ASP:OD1	1:H:154:ASN:N	2.52	0.42
1:I:293:ASP:OD1	1:I:295:LEU:HB3	2.19	0.42
1:B:183:PRO:O	1:B:185:GLN:HG2	2.18	0.42
1:H:225:LEU:HD12	1:I:232:LEU:HD23	2.00	0.42
1:I:123:ARG:CG	1:I:198:VAL:CG1	2.71	0.42
1:C:257:PRO:HG2	1:C:258:TYR:CD2	2.55	0.42
1:J:143:SER:OG	1:J:144:ASP:OD2	2.32	0.42
1:A:253:LEU:HD13	4:A:521:HOH:O	2.20	0.42
1:C:224:TRP:HB2	1:D:281:ILE:HD11	2.01	0.42
1:H:72:TRP:CH2	1:H:140:LEU:HD12	2.54	0.42
1:I:52:GLY:C	1:I:54:LYS:H	2.22	0.42
1:B:35:VAL:HB	1:B:110:PHE:CE1	2.54	0.42
1:C:224:TRP:CB	1:D:281:ILE:HD11	2.49	0.42
1:J:208:PHE:HE1	1:J:248:TYR:CZ	2.38	0.42
1:A:56:LEU:HB3	1:A:94:LEU:HB2	2.02	0.42
1:A:168:THR:HG22	1:A:169:HIS:N	2.34	0.42
1:B:214:LEU:HD22	1:C:274:PHE:CG	2.55	0.42
1:D:256:LEU:HD13	1:D:258:TYR:HE1	1.85	0.42
1:H:105:ARG:HH11	1:H:105:ARG:HD3	1.69	0.42
1:H:224:TRP:CE2	1:H:301:ARG:HB3	2.54	0.42
1:H:269:GLY:O	1:H:273:ILE:HG12	2.19	0.42
1:G:142:PHE:CD2	1:G:191:ILE:HG13	2.55	0.42
1:H:208:PHE:O	1:H:245:TYR:OH	2.35	0.42
1:F:229:SER:OG	1:J:230:GLU:OE2	2.31	0.41
1:H:217:ALA:HA	1:H:220:TRP:CE3	2.55	0.41
3:H:401:MES:H51	3:H:401:MES:H81	1.81	0.41
1:I:72:TRP:HH2	1:I:140:LEU:HD12	1.84	0.41
1:A:29:LEU:HA	1:A:29:LEU:HD23	1.84	0.41
1:B:224:TRP:HB2	1:C:281:ILE:HD11	2.01	0.41
1:C:198:VAL:HG12	1:C:199:ARG:N	2.35	0.41
1:E:38:TYR:CZ	1:E:105:ARG:HD2	2.55	0.41
1:F:185:GLN:NE2	4:F:502:HOH:O	2.15	0.41
1:F:200:ASN:HA	1:F:201:PRO:HD3	1.86	0.41
1:F:292:GLU:O	1:F:294:ASP:N	2.54	0.41
1:H:225:LEU:CD1	1:I:232:LEU:HD23	2.50	0.41
1:J:205:LEU:HD23	1:J:205:LEU:HA	1.88	0.41
1:A:130:LEU:HB3	1:A:191:ILE:HB	2.02	0.41
1:C:288:ALA:O	1:C:291:VAL:HG12	2.19	0.41
1:G:16:VAL:O	1:G:145:ILE:HD12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:127:VAL:O	1:I:128:LEU:HD12	2.20	0.41
1:B:297:ILE:O	1:B:298:GLN:HB2	2.21	0.41
1:B:298:GLN:HG2	1:B:301:ARG:CZ	2.50	0.41
1:C:212:LEU:HB2	1:C:245:TYR:CE2	2.56	0.41
1:E:302:LEU:HD23	1:E:302:LEU:HA	1.88	0.41
1:F:178:LEU:HD23	1:F:178:LEU:HA	1.88	0.41
1:G:168:THR:C	1:G:169:HIS:CD2	2.93	0.41
1:H:260:THR:H	1:H:263:ASP:HB2	1.86	0.41
1:I:95:PHE:HB2	1:I:99:ARG:HG3	2.03	0.41
1:C:175:TYR:HB2	1:C:178:LEU:HD11	2.03	0.41
1:D:127:VAL:O	1:D:128:LEU:HD12	2.20	0.41
1:G:168:THR:O	1:G:169:HIS:CD2	2.74	0.41
1:C:247:PHE:CD2	1:D:247:PHE:CE2	3.08	0.41
1:G:216:ILE:O	1:G:219:SER:HB3	2.21	0.41
1:G:224:TRP:CG	1:H:281:ILE:HD11	2.55	0.41
1:I:123:ARG:CD	1:I:198:VAL:HG12	2.47	0.41
1:D:52:GLY:C	1:D:54:LYS:H	2.24	0.41
1:E:253:LEU:HB3	1:E:254:PRO:HD2	2.03	0.41
1:H:210:LEU:HB3	1:H:211:PRO:HD3	2.03	0.41
3:C:401:MES:H51	3:C:401:MES:H81	1.88	0.41
1:E:279:LEU:HD22	1:E:304:PHE:HE1	1.86	0.41
1:F:159:GLU:OE2	1:G:29:LEU:HD21	2.21	0.41
1:F:250:SER:CB	1:J:252:ILE:HD11	2.50	0.41
1:C:28:THR:HG22	1:C:116:PHE:CZ	2.55	0.41
1:C:246:ALA:HA	1:C:266:ILE:HD13	2.03	0.41
1:F:132:PRO:CG	1:F:140:LEU:HD22	2.51	0.41
1:G:86:ASP:OD1	1:H:84:SER:OG	2.35	0.41
1:J:128:LEU:HB2	1:J:193:VAL:HB	2.02	0.41
1:J:145:ILE:HD13	1:J:191:ILE:HD13	2.03	0.41
1:J:223:PHE:HE2	1:J:304:PHE:CD2	2.39	0.41
1:G:298:GLN:HA	1:G:301:ARG:HG3	2.03	0.41
1:E:297:ILE:HG13	4:E:502:HOH:O	2.21	0.40
1:G:268:ALA:HB1	1:G:308:PHE:HE1	1.85	0.40
1:D:123:ARG:CG	1:D:198:VAL:CG1	2.66	0.40
1:H:224:TRP:CE2	1:H:301:ARG:HD2	2.56	0.40
1:H:232:LEU:O	1:H:235:SER:OG	2.34	0.40
1:I:212:LEU:HD12	1:I:245:TYR:CE2	2.56	0.40
1:G:178:LEU:HA	1:G:178:LEU:HD23	1.79	0.40
1:G:181:VAL:CG1	1:G:185:GLN:HG3	2.51	0.40
1:H:182:GLN:HB2	1:H:183:PRO:CD	2.49	0.40
1:I:297:ILE:HG22	1:I:298:GLN:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:302:LEU:O	1:C:302:LEU:HD23	2.21	0.40
1:D:66:TRP:HB3	1:D:71:LEU:HD23	2.03	0.40
1:D:91:ARG:HB2	1:E:133:PHE:HE2	1.87	0.40
1:F:38:TYR:CZ	1:F:105:ARG:HD2	2.57	0.40
1:G:50:THR:OG1	1:G:52:GLY:O	2.38	0.40
1:H:225:LEU:HD23	1:H:230:GLU:HB3	2.03	0.40
1:A:52:GLY:C	1:A:54:LYS:H	2.25	0.40
1:B:295:LEU:O	1:B:299:ARG:HD3	2.22	0.40
4:B:505:HOH:O	1:C:77:GLU:OE2	2.22	0.40
1:C:223:PHE:HB2	1:C:301:ARG:HG2	2.04	0.40
1:D:308:PHE:C	1:D:308:PHE:CD2	2.95	0.40
1:D:308:PHE:O	1:D:312:GLY:N	2.55	0.40
1:F:212:LEU:HD11	1:F:266:ILE:HG12	2.04	0.40
1:H:56:LEU:HD12	1:H:57:ILE:H	1.87	0.40
1:H:221:SER:OG	1:I:236:PHE:HZ	2.03	0.40
1:I:72:TRP:CH2	1:I:74:PRO:HG3	2.57	0.40
1:I:129:GLU:OE2	1:I:190:ARG:NH1	2.54	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:13:ASP:OD2	1:G:174:ARG:NH2[2_556]	2.16	0.04

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	307/322 (95%)	283 (92%)	22 (7%)	2 (1%)	22 60
1	B	307/322 (95%)	282 (92%)	23 (8%)	2 (1%)	22 60
1	C	307/322 (95%)	282 (92%)	24 (8%)	1 (0%)	41 76

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	307/322 (95%)	284 (92%)	22 (7%)	1 (0%)	41	76
1	E	307/322 (95%)	281 (92%)	24 (8%)	2 (1%)	22	60
1	F	307/322 (95%)	283 (92%)	22 (7%)	2 (1%)	22	60
1	G	307/322 (95%)	282 (92%)	23 (8%)	2 (1%)	22	60
1	H	307/322 (95%)	282 (92%)	24 (8%)	1 (0%)	41	76
1	I	307/322 (95%)	286 (93%)	19 (6%)	2 (1%)	22	60
1	J	307/322 (95%)	282 (92%)	24 (8%)	1 (0%)	41	76
All	All	3070/3220 (95%)	2827 (92%)	227 (7%)	16 (0%)	29	68

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	182	GLN
1	C	182	GLN
1	E	182	GLN
1	F	182	GLN
1	H	182	GLN
1	J	182	GLN
1	A	293	ASP
1	D	182	GLN
1	F	181	VAL
1	G	182	GLN
1	I	181	VAL
1	A	182	GLN
1	B	182	GLN
1	E	181	VAL
1	B	293	ASP
1	G	293	ASP

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	277/284 (98%)	275 (99%)	2 (1%)	84	94
1	B	277/284 (98%)	274 (99%)	3 (1%)	73	90
1	C	277/284 (98%)	275 (99%)	2 (1%)	84	94
1	D	277/284 (98%)	273 (99%)	4 (1%)	67	88
1	E	277/284 (98%)	270 (98%)	7 (2%)	47	79
1	F	277/284 (98%)	275 (99%)	2 (1%)	84	94
1	G	277/284 (98%)	276 (100%)	1 (0%)	91	97
1	H	277/284 (98%)	271 (98%)	6 (2%)	52	81
1	I	277/284 (98%)	274 (99%)	3 (1%)	73	90
1	J	277/284 (98%)	275 (99%)	2 (1%)	84	94
All	All	2770/2840 (98%)	2738 (99%)	32 (1%)	71	90

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	205	LEU
1	A	247	PHE
1	B	202	SER
1	B	295	LEU
1	B	304	PHE
1	C	253	LEU
1	C	308	PHE
1	D	29	LEU
1	D	247	PHE
1	D	258	TYR
1	D	308	PHE
1	E	14	VAL
1	E	29	LEU
1	E	58	VAL
1	E	247	PHE
1	E	258	TYR
1	E	295	LEU
1	E	308	PHE
1	F	295	LEU
1	F	308	PHE
1	G	58	VAL
1	H	58	VAL
1	H	91	ARG
1	H	247	PHE

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Mol	Chain	Res	Type
1	H	258	TYR
1	H	295	LEU
1	H	308	PHE
1	I	258	TYR
1	I	302	LEU
1	I	308	PHE
1	J	247	PHE
1	J	258	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	251	ASN
1	B	251	ASN
1	B	264	GLN
1	C	251	ASN
1	C	284	HIS
1	C	289	ASN
1	D	69	ASN
1	D	125	GLN
1	D	139	GLN
1	D	169	HIS
1	D	185	GLN
1	D	233	GLN
1	D	251	ASN
1	D	285	HIS
1	E	251	ASN
1	F	103	ASN
1	F	233	GLN
1	F	251	ASN
1	G	169	HIS
1	G	251	ASN
1	G	285	HIS
1	H	103	ASN
1	H	251	ASN
1	I	103	ASN
1	I	169	HIS
1	I	251	ASN
1	J	103	ASN
1	J	251	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

14 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	MES	C	401	-	12,12,12	2.26	1 (8%)	14,16,16	2.68	7 (50%)
3	MES	D	401	-	12,12,12	2.13	1 (8%)	14,16,16	2.58	6 (42%)
3	MES	I	401	-	12,12,12	2.20	1 (8%)	14,16,16	2.17	6 (42%)
3	MES	B	401	-	12,12,12	2.37	1 (8%)	14,16,16	2.25	5 (35%)
3	MES	J	401	-	12,12,12	2.25	1 (8%)	14,16,16	2.28	7 (50%)
3	MES	F	403	-	12,12,12	2.21	1 (8%)	14,16,16	2.54	7 (50%)
2	4LE	F	401	-	6,9,9	0.38	0	7,13,13	1.43	1 (14%)
3	MES	A	402	-	12,12,12	2.33	1 (8%)	14,16,16	2.53	7 (50%)
3	MES	A	403	-	12,12,12	2.32	1 (8%)	14,16,16	1.97	6 (42%)
3	MES	G	401	-	12,12,12	2.26	1 (8%)	14,16,16	2.30	7 (50%)
2	4LE	F	402	-	6,9,9	0.50	0	7,13,13	1.35	0
2	4LE	A	401	-	6,9,9	0.67	0	7,13,13	1.73	2 (28%)
2	4LE	E	401	-	6,9,9	0.39	0	7,13,13	1.46	2 (28%)
3	MES	H	401	-	12,12,12	2.28	1 (8%)	14,16,16	2.58	7 (50%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MES	C	401	-	-	5/6/14/14	0/1/1/1
3	MES	D	401	-	-	1/6/14/14	0/1/1/1
3	MES	I	401	-	-	2/6/14/14	0/1/1/1
3	MES	B	401	-	-	4/6/14/14	0/1/1/1
3	MES	J	401	-	-	5/6/14/14	0/1/1/1
3	MES	F	403	-	-	1/6/14/14	0/1/1/1
2	4LE	F	401	-	-	5/8/10/10	-
3	MES	A	402	-	-	3/6/14/14	0/1/1/1
3	MES	A	403	-	-	3/6/14/14	0/1/1/1
3	MES	G	401	-	-	3/6/14/14	0/1/1/1
2	4LE	F	402	-	-	4/8/10/10	-
2	4LE	A	401	-	-	3/8/10/10	-
2	4LE	E	401	-	-	3/8/10/10	-
3	MES	H	401	-	-	4/6/14/14	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	401	MES	C8-S	-7.99	1.66	1.77
3	A	403	MES	C8-S	-7.81	1.66	1.77
3	A	402	MES	C8-S	-7.80	1.66	1.77
3	H	401	MES	C8-S	-7.64	1.66	1.77
3	C	401	MES	C8-S	-7.63	1.66	1.77
3	G	401	MES	C8-S	-7.59	1.66	1.77
3	J	401	MES	C8-S	-7.55	1.66	1.77
3	F	403	MES	C8-S	-7.40	1.67	1.77
3	I	401	MES	C8-S	-7.38	1.67	1.77
3	D	401	MES	C8-S	-7.13	1.67	1.77

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	402	MES	C5-N4-C3	5.33	120.84	108.83
3	H	401	MES	C5-N4-C3	5.26	120.67	108.83
3	C	401	MES	C5-N4-C3	5.16	120.45	108.83
3	F	403	MES	C5-N4-C3	5.10	120.31	108.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	401	MES	C5-N4-C3	5.09	120.28	108.83
3	B	401	MES	C5-N4-C3	5.08	120.25	108.83
3	C	401	MES	O1S-S-C8	4.93	112.85	106.92
3	J	401	MES	C5-N4-C3	4.63	119.26	108.83
3	A	403	MES	C5-N4-C3	4.34	118.61	108.83
3	I	401	MES	C5-N4-C3	4.26	118.42	108.83
3	G	401	MES	C5-N4-C3	4.12	118.10	108.83
3	D	401	MES	O2S-S-C8	3.99	111.72	106.92
3	D	401	MES	O1S-S-C8	3.63	111.29	106.92
3	A	402	MES	C6-C5-N4	-3.57	104.69	110.10
3	H	401	MES	O1S-S-C8	3.57	111.21	106.92
3	D	401	MES	C7-N4-C5	3.57	120.36	111.23
3	F	403	MES	C7-N4-C5	3.48	120.12	111.23
3	H	401	MES	C7-N4-C5	3.44	120.02	111.23
3	C	401	MES	C7-N4-C5	3.40	119.93	111.23
3	G	401	MES	O2S-S-C8	3.40	111.00	106.92
3	A	402	MES	C7-N4-C5	3.36	119.82	111.23
3	G	401	MES	C6-C5-N4	-3.31	105.09	110.10
3	C	401	MES	C7-N4-C3	3.28	119.62	111.23
3	I	401	MES	O1S-S-C8	3.24	110.82	106.92
3	J	401	MES	C6-C5-N4	-3.23	105.20	110.10
3	B	401	MES	O3S-S-C8	3.20	110.94	105.77
3	F	403	MES	C7-N4-C3	3.19	119.40	111.23
3	A	402	MES	C7-N4-C3	3.17	119.34	111.23
3	D	401	MES	C7-N4-C3	3.16	119.32	111.23
3	H	401	MES	C7-N4-C3	3.09	119.14	111.23
3	A	403	MES	O1S-S-C8	3.09	110.64	106.92
3	F	403	MES	O3S-S-C8	3.01	110.64	105.77
3	C	401	MES	C6-C5-N4	-3.00	105.56	110.10
3	H	401	MES	C6-C5-N4	-2.92	105.68	110.10
3	F	403	MES	C6-C5-N4	-2.89	105.73	110.10
2	A	401	4LE	F03-C01-F02	2.84	113.22	106.87
3	G	401	MES	O3S-S-C8	2.81	110.32	105.77
3	G	401	MES	C7-N4-C5	2.79	118.38	111.23
3	I	401	MES	O3S-S-C8	2.73	110.18	105.77
3	J	401	MES	C7-N4-C3	2.72	118.19	111.23
3	J	401	MES	O3S-S-C8	2.71	110.15	105.77
3	F	403	MES	O1S-S-C8	2.70	110.17	106.92
3	G	401	MES	C7-N4-C3	2.69	118.11	111.23
3	F	403	MES	C2-C3-N4	-2.67	106.05	110.10
3	H	401	MES	C2-C3-N4	-2.62	106.13	110.10
3	H	401	MES	O3S-S-C8	2.62	110.00	105.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	401	MES	C7-N4-C5	2.59	117.86	111.23
3	A	402	MES	O1S-S-C8	2.58	110.02	106.92
3	A	402	MES	C2-C3-N4	-2.58	106.19	110.10
3	J	401	MES	C7-N4-C5	2.52	117.67	111.23
3	I	401	MES	C7-N4-C5	2.50	117.62	111.23
3	J	401	MES	O1S-S-C8	2.49	109.92	106.92
3	C	401	MES	C2-C3-N4	-2.49	106.33	110.10
2	E	401	4LE	F01-C01-C02	-2.44	106.16	111.81
3	J	401	MES	C2-C3-N4	-2.43	106.42	110.10
3	B	401	MES	C7-N4-C3	2.41	117.39	111.23
3	I	401	MES	C6-C5-N4	-2.40	106.46	110.10
3	B	401	MES	O1S-S-C8	2.35	109.75	106.92
3	I	401	MES	C7-N4-C3	2.35	117.25	111.23
2	F	401	4LE	F02-C01-C02	-2.30	106.46	111.81
3	C	401	MES	O3S-S-C8	2.24	109.39	105.77
3	A	403	MES	C7-N4-C5	2.23	116.95	111.23
3	A	403	MES	O3S-S-C8	2.23	109.38	105.77
3	G	401	MES	C2-C3-N4	-2.18	106.80	110.10
3	A	403	MES	O2S-S-C8	2.18	109.54	106.92
2	A	401	4LE	F01-C01-C02	-2.17	106.77	111.81
3	A	403	MES	C6-C5-N4	-2.15	106.85	110.10
3	D	401	MES	C6-C5-N4	-2.10	106.92	110.10
2	E	401	4LE	F03-C01-F02	2.08	111.51	106.87
3	A	402	MES	O2S-S-C8	2.04	109.37	106.92

There are no chirality outliers.

All (46) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	4LE	F01-C01-C02-O01
2	A	401	4LE	F02-C01-C02-O01
2	A	401	4LE	F03-C01-C02-O01
2	E	401	4LE	F01-C01-C02-O01
2	E	401	4LE	F02-C01-C02-O01
2	E	401	4LE	F03-C01-C02-O01
2	F	401	4LE	F01-C01-C02-O01
2	F	401	4LE	F02-C01-C02-O01
2	F	401	4LE	F03-C01-C02-O01
2	F	401	4LE	F04-C03-O01-C02
2	F	401	4LE	F05-C03-O01-C02
2	F	402	4LE	F01-C01-C02-O01
2	F	402	4LE	F02-C01-C02-O01

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Mol	Chain	Res	Type	Atoms
2	F	402	4LE	F03-C01-C02-O01
2	F	402	4LE	F05-C03-O01-C02
3	A	402	MES	C8-C7-N4-C5
3	A	403	MES	C7-C8-S-O1S
3	A	403	MES	C7-C8-S-O2S
3	B	401	MES	N4-C7-C8-S
3	C	401	MES	N4-C7-C8-S
3	G	401	MES	N4-C7-C8-S
3	H	401	MES	C7-C8-S-O1S
3	I	401	MES	C8-C7-N4-C3
3	J	401	MES	C7-C8-S-O2S
3	J	401	MES	C7-C8-S-O3S
3	B	401	MES	C7-C8-S-O3S
3	H	401	MES	C7-C8-S-O3S
3	A	403	MES	C7-C8-S-O3S
3	A	402	MES	C8-C7-N4-C3
3	C	401	MES	C8-C7-N4-C3
3	D	401	MES	C8-C7-N4-C3
3	F	403	MES	C8-C7-N4-C3
3	G	401	MES	C8-C7-N4-C5
3	H	401	MES	C8-C7-N4-C3
3	I	401	MES	C8-C7-N4-C5
3	J	401	MES	C8-C7-N4-C3
3	C	401	MES	C7-C8-S-O3S
3	A	402	MES	C7-C8-S-O1S
3	B	401	MES	C7-C8-S-O1S
3	B	401	MES	C7-C8-S-O2S
3	C	401	MES	C7-C8-S-O1S
3	C	401	MES	C7-C8-S-O2S
3	H	401	MES	C7-C8-S-O2S
3	J	401	MES	C7-C8-S-O1S
3	G	401	MES	C8-C7-N4-C3
3	J	401	MES	C8-C7-N4-C5

There are no ring outliers.

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	401	MES	1	0
3	J	401	MES	1	0
2	F	401	4LE	1	0
3	G	401	MES	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	402	4LE	1	0
3	H	401	MES	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	309/322 (95%)	-0.22	9 (2%)	51	23	62, 93, 151, 241	0
1	B	309/322 (95%)	-0.26	10 (3%)	47	20	55, 80, 175, 227	0
1	C	309/322 (95%)	-0.26	7 (2%)	60	31	53, 83, 179, 228	0
1	D	309/322 (95%)	-0.11	13 (4%)	36	14	51, 78, 171, 249	0
1	E	309/322 (95%)	-0.14	12 (3%)	39	15	58, 89, 169, 236	0
1	F	309/322 (95%)	-0.23	12 (3%)	39	15	59, 98, 166, 264	0
1	G	309/322 (95%)	-0.25	8 (2%)	56	27	54, 81, 149, 231	0
1	H	309/322 (95%)	-0.11	17 (5%)	25	9	59, 88, 175, 256	0
1	I	309/322 (95%)	-0.16	14 (4%)	33	12	58, 86, 175, 236	0
1	J	309/322 (95%)	-0.05	15 (4%)	29	11	63, 98, 190, 244	0
All	All	3090/3220 (95%)	-0.18	117 (3%)	40	16	51, 88, 174, 264	0

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	180	SER	9.8
1	D	181	VAL	8.2
1	D	179	SER	7.9
1	I	179	SER	6.6
1	B	290	GLY	6.1
1	E	289	ASN	6.0
1	D	182	GLN	6.0
1	D	178	LEU	5.5
1	I	154	ASN	5.4
1	H	181	VAL	5.3
1	J	289	ASN	5.1
1	F	179	SER	5.1
1	E	179	SER	4.9

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Mol	Chain	Res	Type	RSRZ
1	J	305	PRO	4.8
1	J	306	LEU	4.8
1	E	290	GLY	4.8
1	B	179	SER	4.8
1	G	315	LEU	4.7
1	F	287	GLN	4.7
1	J	287	GLN	4.4
1	J	154	ASN	4.0
1	J	290	GLY	3.9
1	I	153	ASP	3.8
1	I	287	GLN	3.7
1	B	289	ASN	3.7
1	J	318	ARG	3.5
1	H	289	ASN	3.5
1	H	180	SER	3.5
1	I	317	ILE	3.5
1	E	318	ARG	3.3
1	I	157	ILE	3.3
1	H	317	ILE	3.3
1	F	316	VAL	3.3
1	H	288	ALA	3.2
1	E	288	ALA	3.2
1	J	156	GLU	3.1
1	D	289	ASN	3.1
1	I	185	GLN	3.1
1	D	157	ILE	3.1
1	F	244	ALA	3.0
1	E	157	ILE	3.0
1	H	179	SER	3.0
1	B	315	LEU	2.9
1	D	153	ASP	2.9
1	I	318	ARG	2.9
1	D	177	HIS	2.9
1	D	183	PRO	2.8
1	H	291	VAL	2.8
1	H	185	GLN	2.8
1	J	237	THR	2.8
1	G	157	ILE	2.8
1	I	180	SER	2.8
1	H	318	ARG	2.8
1	F	288	ALA	2.8
1	A	54	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	F	182	GLN	2.7
1	A	53	ASP	2.7
1	A	179	SER	2.7
1	C	316	VAL	2.7
1	E	287	GLN	2.6
1	E	291	VAL	2.6
1	G	312	GLY	2.6
1	A	178	LEU	2.6
1	G	311	ILE	2.6
1	J	153	ASP	2.6
1	H	183	PRO	2.6
1	C	314	VAL	2.6
1	I	183	PRO	2.6
1	H	182	GLN	2.6
1	F	240	LEU	2.6
1	F	299	ARG	2.5
1	I	182	GLN	2.5
1	B	291	VAL	2.5
1	G	295	LEU	2.5
1	C	240	LEU	2.5
1	B	244	ALA	2.5
1	E	237	THR	2.4
1	A	296	LEU	2.4
1	C	243	VAL	2.4
1	G	240	LEU	2.4
1	D	154	ASN	2.4
1	J	240	LEU	2.4
1	I	237	THR	2.4
1	J	303	ALA	2.4
1	A	244	ALA	2.4
1	J	241	THR	2.4
1	H	314	VAL	2.4
1	B	237	THR	2.3
1	H	292	GLU	2.3
1	B	296	LEU	2.3
1	A	287	GLN	2.3
1	D	288	ALA	2.3
1	F	237	THR	2.2
1	G	241	THR	2.2
1	C	315	LEU	2.2
1	F	178	LEU	2.2
1	G	287	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	289	ASN	2.2
1	H	174	ARG	2.2
1	H	311	ILE	2.2
1	B	294	ASP	2.2
1	A	152	ILE	2.2
1	E	241	THR	2.2
1	F	241	THR	2.2
1	I	286	ARG	2.2
1	E	49	LYS	2.2
1	H	241	THR	2.2
1	C	317	ILE	2.1
1	H	244	ALA	2.1
1	A	286	ARG	2.1
1	J	157	ILE	2.1
1	B	241	THR	2.1
1	C	318	ARG	2.1
1	E	154	ASN	2.1
1	J	291	VAL	2.1
1	I	290	GLY	2.1
1	D	311	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MES	C	401	12/12	0.80	0.19	109,123,138,142	0
3	MES	I	401	12/12	0.81	0.26	125,131,157,160	0
3	MES	J	401	12/12	0.83	0.21	146,154,166,168	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MES	F	403	12/12	0.84	0.15	117,127,146,150	0
3	MES	A	402	12/12	0.85	0.18	106,120,174,174	0
3	MES	A	403	12/12	0.85	0.15	127,135,140,142	0
3	MES	D	401	12/12	0.86	0.22	115,125,128,128	0
3	MES	H	401	12/12	0.87	0.17	116,122,150,150	0
3	MES	B	401	12/12	0.93	0.09	108,116,132,136	0
3	MES	G	401	12/12	0.94	0.21	108,117,138,140	0
2	4LE	E	401	10/10	0.95	0.42	109,119,146,148	0
2	4LE	A	401	10/10	0.97	0.30	116,119,131,140	0
2	4LE	F	402	10/10	0.97	0.30	109,117,122,133	0
2	4LE	F	401	10/10	0.98	0.36	119,120,127,146	0

6.5 Other polymers (i)

There are no such residues in this entry.